

Universality in the partially anisotropic three-dimensional Ising lattice

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Abstract

Using transfer-matrix extended phenomenological renormalization-group methods the critical properties of spin-1/2 Ising model on a simple-cubic lattice with partly anisotropic coupling strengths $\vec{J} = (J', J', J)$ are studied. Universality of both fundamental critical exponents y_t and y_h is confirmed. It is shown that the critical finite-size scaling amplitude ratios $U = A_{\chi^{(4)}} A_{\kappa} / A_{\chi}^2$, $Y_1 = A_{\kappa''} / A_{\chi}$, and $Y_2 = A_{\kappa^{(4)}} / A_{\chi^{(4)}}$ are independent of the lattice anisotropy parameter $\Delta = J' / J$. By this for the last above invariant of the three-dimensional Ising universality class we give the first quantitative estimate: $Y_2 \simeq 2.013$ (shape $L \times L \times \infty$, periodic boundary conditions in both transverse directions).

PACS numbers: 05.50.+q, 05.70.Jk, 64.60.Fr, 75.10.Hk

1 Introduction

The phenomenological renormalization-group (RG) method in which the transfer-matrix technique and finite-size scaling (FSS) ideas are combined is a powerful tool for investigation of critical properties in different two-dimensional systems [1, 2]. Unfortunately, its application in three and more dimensions is sharply retarded due to huge sizes of transfer matrices which arise in approximations of d -dimensional lattices by $L^{d-1} \times \infty$ subsystems.

Indeed, even in the simplest case of systems with only two states of a site (a spin- $\frac{1}{2}$ Ising model) the order of transfer matrix in three dimensions ($d = 3$) increases according to the law 2^{L^2} (instead of the essentially more sparing law 2^L in two dimensions). Hence, for the cluster $3 \times 3 \times \infty$ it is needed to solve the eigenproblem of the transfer matrix 512×512 , for the $4 \times 4 \times \infty$ subsystem — $65\,536 \times 65\,536$, and for the $5 \times 5 \times \infty$ cluster it is required to find the eigenvalues and eigenvectors of dense matrices with huge sizes of $33\,554\,432$ by $33\,554\,432$.

One can now solve the full eigenproblem for the transfer matrices of Ising parallelepipeds $L \times L \times \infty$ with the side length $L \leq 4$. Our aim in this paper is to use such solutions with the largest effect and extract as much as possible accurate information about physical properties of the bulk system.

The ordinary phenomenological RG is based on the FSS equations for correlation lengths [1, 2]. However, it is known [3, 4, 5] that the phenomenological RG can be built up using other quantities with a power divergence at the phase-transition point. It is remarkable that the such modified renormalizations can provide more precise results by the same sizes of subsystems [6].

In this paper we calculate the values of different invariants of the 3D Ising universality class and discuss their universal and extrauniversal properties.

2 Basic equations

Start from the ordinary FSS equations [1, 2] for the inverse correlation length $\kappa_L(t, h)$ and singular part of the dimensionless free-energy density $f_L^s(t, h)$, but we write them out for the derivatives with respect to the reduced temperature $t = (T - T_c)/T_c$ and external field h :

$$\kappa_L^{(m,n)}(t, h) = b^{my_t + ny_h - 1} \kappa_{L/b}^{(m,n)}(t', h') \quad (1)$$

and

$$f_L^{s(m,n)}(t, h) = b^{my_t + ny_h - d} f_{L/b}^{s(m,n)}(t', h'). \quad (2)$$

Here $\kappa_L^{(m,n)}(t, h) = \partial^{m+n} \kappa_L / \partial t^m \partial h^n$ and the same for $f_L^{s(m,n)}$; y_t and y_h are, respectively, the thermal and magnetic critical exponents of the system; $b = L/L'$ is the rescaling factor. Deriving Eqs. (1) and (2) we used a linearized form of RG equations $t' \simeq b^{y_t} t$ and $h' \simeq b^{y_h} h$.

In the traditional phenomenological RG theory [1, 2], Eq. (1) with $m = n = 0$ is considered as an RG mapping $(t, h) \rightarrow (t', h')$ for a cluster pair (L, L') . By this, the

critical temperature T_c is estimated from the equation

$$L\kappa_L(T_c) = L'\kappa_{L'}(T_c). \quad (3)$$

Phenomenological renormalization $(t, h) \rightarrow (t', h')$ can be also realized by using any of the relations (1) and (2) or their combination. It has been shown by the author [6] that some of such extended renormalizations lead to more rapid convergence in L than the standard phenomenological RG transformation. In particular, test examples on the fully isotropic systems [6] exhibited that the relations

$$\frac{\kappa_L''}{L^{d-1}\chi_L} \Big|_{T_c} = \frac{\kappa_{L'}''}{(L')^{d-1}\chi_{L'}} \Big|_{T_c} \quad (4)$$

and

$$\frac{\chi_L^{(4)}}{L^d\chi_L^2} \Big|_{T_c} = \frac{\chi_{L'}^{(4)}}{(L')^d\chi_{L'}^2} \Big|_{T_c} \quad (5)$$

locate T_c more accurately in comparison with the ordinary RG equation (3). In the relations (4) and (5), the derivative $\kappa_L'' = \partial^2 \kappa_L / \partial h^2$, the zero-field susceptibility $\chi_L = f_L^{s(0,2)}$, and the nonlinear susceptibility $\chi_L^{(4)} = f_L^{s(0,4)}$ can be evaluated by standard formulas via the eigenvalues and eigenvectors of transfer matrices (see, e. g., [7, 8, 9]).

To get the thermal critical exponent y_t we applied two approaches. Firstly, we used again the standard finite-size expression

$$y_t = \frac{\ln[L\dot{\kappa}_L/(L'\dot{\kappa}_{L'})]}{\ln(L/L')} \quad (6)$$

which follows from Eq. (1) by $m = 1$, $n = 0$; $\dot{\kappa}_L = \partial \kappa_L / \partial t$. Secondly, we took the formula

$$y_t = \frac{\kappa_{L'}\dot{\kappa}_L - \kappa_L\dot{\kappa}_{L'}}{(\kappa_L\kappa_{L'}\dot{\kappa}_L\dot{\kappa}_{L'})^{1/2} \ln(L/L')}. \quad (7)$$

This expression is a direct sequence of the well-known Roomany-Wyld approximant to the Callan-Symanzik β -function [2].

To calculate the magnetic critical exponent y_h we also used two ways:

$$y_h = \frac{d}{2} + \frac{\ln(\chi_L/\chi_{L'})}{2 \ln(L/L')} \quad (8)$$

and

$$y_h = \frac{1}{2} + \frac{\ln(\kappa_L''/\kappa_{L'}'')}{2 \ln(L/L')} \quad (9)$$

[these finite-size relations follow from Eqs. (1) and (2)].

In addition, we calculated the universal ratios of critical FSS amplitudes. Such a kind of the ratios can be identified from the Privman-Fisher functional expressions [10]. For the discussed anisotropic systems, they read [8]

$$\kappa_L(t, h) = L^{-1} G_0 \mathcal{K}(C_1 t L^{y_t}, C_2 h L^{y_h}) \quad (10)$$

and

$$f_L^s(t, h) = L^{-d} G_0 \mathcal{F}(C_1 t L^{y_t}, C_2 h L^{y_h}). \quad (11)$$

Scaling functions $\mathcal{K}(x_1, x_2)$ and $\mathcal{F}(x_1, x_2)$ are the same within the limits of a given universality class but they may depend on the boundary conditions and the subsystem shape (a cube, infinitely long parallelepipeds, etc.). Thus, all nonuniversality *including the lattice anisotropy parameter* Δ is absorbed in the geometry prefactor G_0 and metric coefficients C_1 and C_2 . The critical amplitude ratios from which the parameters G_0 , C_1 , and C_2 drop out should be extrauniversal. In particular, the amplitude combinations

$$U = \frac{A_{\chi^{(4)}} A_{\kappa}}{A_{\chi}^2} = \frac{\kappa_L \chi_L^{(4)}}{L^{d-1} \chi_L^2} \quad (12)$$

(Binder-like ratio for the spatially anisotropic systems),

$$Y_1 = \frac{A_{\kappa''}}{A_{\chi}} = \frac{\kappa_L''}{L^{d-1} \chi_L}, \quad (13)$$

and

$$Y_2 = \frac{A_{\kappa^{(4)}}}{A_{\chi^{(4)}}} = \frac{\kappa_L^{(4)}}{L^{d-1} \chi_L^{(4)}} \quad (14)$$

are expected to be not depend on the lattice anisotropy parameter $\Delta = J'/J$.

3 Results and discussion

In the present paper we carried out calculations for the subsystems $L \times L \times \infty$ with $L = 3$ and 4. To avoid undesirable surface effects the periodic boundary conditions have been imposed in both transverse directions of parallelepipeds $L \times L \times \infty$. Thus, the transfer matrices for which the eigenproblems was solved were dense matrices of sizes up to $65\,536 \times 65\,536$. To solve the eigenproblem we took into account the internal and lattice symmetries of subsystems and used the block-diagonalization method (see, e. g., [9, 7]). Calculations were performed on an 800 MHz Pentium III PC running the FreeBSD operating system.

3.1 Critical temperature

The critical temperature estimates coming from solutions of the transcendental equations (4) and (5) are collected in Table 1.

In the purely isotropic case ($J' = J$) there are high precision numerical estimates for the critical point of the 3D Ising model. The most precise values for it have been obtained by Monte Carlo simulations [11, 12]; $K_c = 0.221\,654\,59(10)$, i. e. $k_B T_c / J = 1/K_c = 4.511\,5240(21)$.

Inspecting Table 1 one can see that the estimates for $J' = J$ which follow from Eq. (4) and (5) are the lower and upper bounds respectively. By this, their mean value has the accuracy of 0.01%. Note also that our mean estimate is better than the

value $k_B T_c/J = 4.53371$ obtained in Ref. [13] (see also [14]) for the fully isotropic lattice by using the ordinary phenomenological renormalization of the bars with $L = 4$ and 5.

Discuss now the anisotropic case. Here there is well-known exact asymptotic formula for the critical temperature [15]

$$(k_B T_c/J)_{\text{asym}} = 2/[\ln(J/2J') - \ln \ln(J/2J') + O(1)] \quad (15)$$

as $J'/J \rightarrow 0$. It is a direct consequence of the molecular-field approximation in which the linear Ising chain is taken as a cluster.

Unfortunately, simple formula (15) yields considerable errors in the region $10^{-3} \leq J'/J \leq 1$. Its modifications in spirit of Ref. [16], $k_B T_c/J \approx 2/[\ln(J/J') - \ln \ln(J/J')]$, lead to a loss of monotonous convergence when J'/J varies from unity to zero.

We choose infinitely long clusters $L \times L \times \infty$ stretched in a lattice direction with the dominant interaction J . Such a cluster geometry reflects the physical situation in the system. Therefore one may expect more precise results for the critical temperature as the anisotropy of the quasi-one-dimensional lattice increases. We may also expect the monotonous convergence for the estimates from Eq. (4) and (5) because there are must be physical reasons (finite length of clusters in the longitudinal direction, etc.) for the non-monotonous or oscillatory character of behavior; they are absent in our approximations. That is, if Eq. (4) yields the lower bound in the most unfavorable case $J' = J$ then it should preserve such behavior for all $J' < J$. Similar arguments are valid for the estimates following from Eq. (5); these estimates are upper.

Note that the mean values from Table 1 are better not only than the estimates of $k_B T_c/J$ calculated with the (3,4) cluster pair by the standard phenomenological RG method, but than their improvements found by means of three-point extrapolations from the sizes $L = 2, 3$, and 4 to the bulk limit [17].

In the range $10^{-2} \leq J'/J \leq 1$, there are also the data for the critical temperature of a simple-cubic Ising lattice which were extracted from the Padé-approximant analysis of the high-temperature series [18]. For $J' = J$ according to these data, $k_B T_c/J = 4.5106$ that is lower by 0.014% in comparison with the results of Ref. [12]. For $J'/J = 0.1$ the authors of Ref. [18] found the value $k_B T_c/J = 1.343$. This quantity overestimates somewhat the mean value from Table 1. At last, for $J'/J = 0.01$ the series method [18] yields $k_B T_c/J = 0.65$ that goes out of our lower bound. This is not surprising because the calculations based on the high-temperature series rapidly deteriorate owing to the very limited number (≤ 11) of terms available in such series for the anisotropic lattices.

So, we may treat the values found from Eqs. (4) and (5) as lower and upper bounds on the real critical temperature. Their mean value for each J'/J yields the best estimate which we achieve in this paper for the reduced critical temperature $k_B T_c/J$ (the last column in Table 1). By this, its absolute error is not larger in any case than the half difference of the corresponding upper and lower bounds. Using data from Table 1 we establish that the relative errors for $k_B T_c/J$ monotonically decrease from 0.72% to 0.14% as J'/J goes from 1 to 10^{-3} .

3.2 Invariants of the 3D Ising universality class

Taking the improved estimates for the critical temperature of anisotropic simple-cubic lattice we calculate now some invariants of the three-dimensional Ising model universality class.

3.2.1 Critical exponents

According to the RG theory, critical exponents are determined entirely by a fixed point and do not depend on the lattice anisotropy. For a three-dimensional Ising model the universality of critical exponents has been confirmed for $\Delta \in [0.2, 5]$ by the high-temperature series calculations [19].

At present, the most precise estimates of critical exponents are provided by the high-temperature expansions for ordinary models [20] and for models with improved potentials characterized by suppressed leading scaling corrections [21]. For the 3D Ising lattice (fully isotropic) these methods yield $\nu = 0.630\,12(16)$ and $\gamma = 1.2373(2)$. Hence, $y_t = 1/\nu = 1.5870(4)$ and $y_h = (d + \gamma/\nu)/2 = 2.481\,80(18)$.

In Table 2 we report our estimates for the critical exponents y_t and y_h . It follows from those data that when the lattice anisotropy parameter Δ varies in three orders (from unity to 10^{-3}), the estimates of critical exponents are changed only on a few per cent or less. In particular, calculations by Eqs. (6) and (7) with the cluster pair (3, 4) yield respectively $y_t = 1.47\{6\}$ and $y_t = 1.60\{7\}$. (Here and below, the numbers in curly brackets are dispersions of averages over the lattice anisotropy parameter Δ .) Their variations are over the range 4 – 4.4%. Similar calculations of the magnetic critical exponent carried out by use of Eqs. (8) and (9) also with the pair (3, 4) leads to $y_h = 2.586\{5\}$ and $y_h = 2.579\{5\}$, correspondingly. Relative dispersions of these estimates are about 0.2%.

Thus, our calculations confirm the universality of both critical exponents in an essentially wider range of Δ than it was done in earlier investigations. Systematic errors of the achieved estimates arise due to small sizes, L , of subsystems used.

3.2.2 Critical FSS amplitude ratios

Critical amplitudes are determined by scaling functions. As a result, their “universal ratios” like $A_{\kappa(4)}/A_{\chi(4)} = \mathcal{K}^{(0,4)}(0, 0)/\mathcal{F}^{(0,4)}(0, 0)$ depend, generally speaking, upon the lattice anisotropy because it can change the shape of subsystems. But in the case of parallelepipeds $L^{d-1} \times \infty$ with unchanged (between themselves) transverse coupling constants the shape of a sample (all its aspect ratios) will be independent of the interaction in longitudinal direction. Such a kind of the universality is studied here.

Table 3 contains results of our calculations for the critical FSS amplitude ratios $U = A_{\chi(4)}A_{\kappa}/A_{\chi}^2$, $Y_1 = A_{\kappa''}/A_{\chi}$, and $Y_2 = A_{\kappa(4)}/A_{\chi(4)}$. Calculations have been carried out for $\Delta \in [10^{-3}, 1]$ by use of a cyclic cluster $4 \times 4 \times \infty$.

In accord with data of Table 3, the average ratio $U = 4.900\{3\}$. Hence, when the anisotropy parameter Δ varies in three orders, this quantity changes only on 0.06%. With such accuracy we may consider the given ratio as a constant. In the

case of fully isotropic lattice, $A_\kappa = 1.26(5)$ and $A_{\chi^{(4)}}/A_\chi^2 = 3.9(2)$ [8] and therefore $A_{\chi^{(4)}}A_\kappa/A_\chi^2 = 4.9(5)$. Our values of U from Table 3 are in good agreement with this estimate.

It follows from Table 3 that $Y_1 = A_{\kappa''}/A_\chi = 1.759(2)$. Hence, the constancy of this universal amplitude ratio is estimated at least as a few times 10^{-3} . Our average value for Y_1 agrees well with the estimate for the isotropic lattice, $A_{\kappa''}/A_\chi = 1.749(6)$ [8].

According to data of Table 3 the amplitude ratio $Y_2 = A_{\kappa^{(4)}}/A_{\chi^{(4)}} = 2.0133\{6\}$. Thus, this quantity is most stable out of all invariants of the 3D Ising universality class which were investigated in the paper. Note that we are not aware of any quantitative estimates for the $A_{\kappa^{(4)}}/A_{\chi^{(4)}}$.

4 Conclusions

In this paper the large-scale transfer-matrix computations have been carried out. Application of the extended phenomenological RG schemes allowed to find the tight limits on the critical temperature in the anisotropic simple-cubic Ising lattice and improve the available estimates for it.

We calculated the thermal and magnetic critical exponents. Our results confirm the universality of y_t within $4 - 4.4\%$ and of y_h within 0.2% over a remarkably wider range of Δ ($10^{-3} \leq \Delta \leq 1$) than in Ref. [19].

Finally, the presented results give an obvious evidence that the critical FSS amplitude ratios $U = A_{\chi^{(4)}}A_\kappa/A_\chi^2$, $Y_1 = A_{\kappa''}/A_\chi$, and $Y_2 = A_{\kappa^{(4)}}/A_{\chi^{(4)}}$ do not depend on the lattice anisotropy parameter $\Delta = J'/J$ with accuracies at least 0.1% . We give likely for the first time in the literature an estimate for the universal quantity Y_2 .

Acknowledgment

This work was supported by the Russian Foundation for Basic Research under project 03-02-16909.

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Table 1: Lower and upper bounds on the critical temperature and their mean values (improved estimates of $k_B T_c/J$) in the 3D sc spin- $\frac{1}{2}$ Ising lattice vs $\Delta = J'/J$. Calculations with a cluster pair (3, 4).

| Δ | Eq.(4) | Eq.(5) | mean |
|----------|------------|------------|------------|
| 1.0 | 4.47965814 | 4.54424309 | 4.51195062 |
| 0.5 | 2.91008665 | 2.94295713 | 2.92652189 |
| 0.1 | 1.33649605 | 1.34570054 | 1.34109829 |
| 0.05 | 1.03544938 | 1.04144927 | 1.03844933 |
| 0.01 | 0.65054054 | 0.65323146 | 0.65188600 |
| 0.005 | 0.55440490 | 0.55643112 | 0.55541801 |
| 0.001 | 0.40743000 | 0.40859011 | 0.40801006 |

Table 2: Estimates of the thermal and magnetic critical exponents by different values of $\Delta = J'/J$. Calculations with a cluster pair (3, 4).

| Δ | $k_B T_c/J$ | y_t | | y_h | |
|----------|-------------|-----------|-----------|-----------|-----------|
| | | Eq.(6) | Eq.(7) | Eq.(8) | Eq.(9) |
| 1.0 | 4.51195062 | 1.5760695 | 1.7246286 | 2.5971647 | 2.5886128 |
| 0.5 | 2.92652189 | 1.5256373 | 1.6636718 | 2.5902006 | 2.5819462 |
| 0.1 | 1.34109829 | 1.4700811 | 1.5972576 | 2.5843305 | 2.5766511 |
| 0.05 | 1.03844933 | 1.4533899 | 1.5791439 | 2.5836720 | 2.5761101 |
| 0.01 | 0.65188600 | 1.4236178 | 1.5480583 | 2.5832982 | 2.5758028 |
| 0.005 | 0.55541801 | 1.4141719 | 1.5383503 | 2.5832029 | 2.5757888 |
| 0.001 | 0.40801006 | 1.3984754 | 1.5222765 | 2.5834573 | 2.5757953 |
| | | 1.47{6} | 1.60{7} | 2.586{5} | 2.579{5} |

Table 3: Estimates of the universal critical FSS amplitude ratios $U = A_{\chi^{(4)}} A_{\kappa} / A_{\chi}^2$, $Y_1 = A_{\kappa^{(2)}} / A_{\chi}$, and $Y_2 = A_{\kappa^{(4)}} / A_{\chi^{(4)}}$ for the Ising system with the cylindrical geometry $L \times L \times \infty$ and periodic boundary conditions. Data for $L = 4$.

| Δ | $k_B T_c / J$ | U | Y_1 | Y_2 |
|----------|---------------|-----------|-----------|-----------|
| 1.0 | 4.51195062 | 4.8956599 | 1.7550004 | 2.0146443 |
| 0.5 | 2.92652189 | 4.8967625 | 1.7572512 | 2.0136519 |
| 0.1 | 1.34109829 | 4.9011909 | 1.7596003 | 2.0129829 |
| 0.05 | 1.03844933 | 4.9014406 | 1.7597697 | 2.0129285 |
| 0.01 | 0.65188600 | 4.9015375 | 1.7598563 | 2.0128977 |
| 0.005 | 0.55541801 | 4.9015529 | 1.7598646 | 2.0128953 |
| 0.001 | 0.40801006 | 4.9015782 | 1.7598732 | 2.0128938 |
| | | 4.900{3} | 1.759{2} | 2.0133{6} |